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Abstract

From 1995-2000, researchers at The University of Texas at Austin and the University of Wisconsin, Madison investigated and demonstrated new, intelligent manufacturing processes for growing epitaxial silicon alloy thin films that employ input from *in situ* optical process sensors to maintain precise control of film composition and thickness. The research team accomplished what was set forth in the original proposal. Significant progress was made in understanding the fundamental chemistry and physics of thin alloy films that affects the sensor operation and growth models, in developing and implementing state estimation and model predictive control techniques, in advancing optical sensors that can provide a complete description of the film properties, and in the design and demonstration of strained SiGe/Si and SiGeC/Si heterostructures with significant device performance enhancements over Si-based devices.

Accomplishments

The most significant accomplishment is the demonstration of a closed-loop controller that recognized and corrected large process disturbances to grow complex $\text{Si}_{1-x}\text{Ge}_x$ alloy films. On-line spectroscopic ellipsometry tracks composition and thickness using state estimation theory. An extended Kalman filter utilizes process and sensor models and estimates film growth rate and composition in real time. The ellipsometer measurements are utilized to update the optimization problem solved by the regulator that controls the reactor variables (gas flow rates, growth temperature and reactor pressure). Feedback from the optical sensor rejects unmeasured disturbances and eliminates run-to-run variability allowing for precise control over film quality.

University researchers advanced the nonlinear and linear sensors that are key to any intelligent manufacturing process. Nonlinear spectroscopic second harmonic generation spectroscopy was explored as a surface-specific-probe that complements the diagnostic capabilities of linear spectroscopic ellipsometry, and has the added advantage of using a nearly identical optical configuration. Researchers developed a method of acquiring broadband second harmonic generation spectra in a few seconds by using a ~ 10 fs fundamental pulse so nonlinear data could be collected as quickly as ellipsometric data. Nonlinear spectroscopy was shown to be effective at monitoring dopant concentrations, which affords, for the first time, the ability to monitor this property *in situ*.

Finally, researchers investigated planar and vertical p-type MOSFETs to exploit mobility enhancements in the strained SiC and SiGeC systems; planar $0.5\ \mu\text{m}$ SiC/Si and SiGeC PMOSFETs were demonstrated exhibiting 40 to 50 % drive current enhancements over bulk silicon. Vertical PMOSFETs with sub 100nm channel lengths were designed and fabricated to overcome drain induced barrier lowering (DIBL) and punchthrough. These structures suppress DIBL and permit the drive current and off-state leakage current to be separately optimized, and demonstrate a clear path to overcome many of the challenges sub 100nm devices will face.

Impact

The greatest impact of this work to-date has been in the *in situ* sensor effort and silicon-alloy devices. The fundamental science and engineering that this program developed was communicated in archival journal articles, making the work available to a wide audience of scientists and engineers who can adapt it to different systems. The overarching focus of the program was an intelligent manufacturing process for silicon and silicon-alloy epitaxy. This was completed at the very end of the research program and it is too early to assess if the

manufacturing community will adopt it. A production tool vendor would need to dedicate optical access and additional sensors on single wafer epitaxy reactors for the intelligent manufacturing process to be widely adapted.

This research advanced the "state-of-the-art" in chemical vapor deposition reactor control and operation for epitaxy of silicon-alloy films. We used Si/Ge alloy films to demonstrate our results; however given a new electronic device structure with a new CVD film alloy profile, the new reactor operating policy that manufactures the film profile can be determined. Current industrial practice involves trial and error recipe determination in which new device films are developed and characterized by growing under different "recipes" of processing conditions. The flowrates of precursor gases and reactor temperature and pressure profiles are determined from previous experience with films of similar characteristics and experimental trial and error. The advantages of this approach are that it has a proven track record. The disadvantages are that fundamental understanding does not increase with experience level, novel new device films are not well predicted by past experience, and the experimental effort is expensive and time consuming. It is expected that new device structures will require alloy profiles of several different materials including dopants and it will prove increasingly difficult to determine proper operating profiles through direct trial and error experiments. In our work, kinetic models of the gas phase and surface chemistry were developed and coupled to reactor models for the new CVD process of interest. Most of the model parameters are identified from available kinetic studies and only a few are fit to measurements taken from the reactor used for device manufacture. The model is then used to determine the best operating policy that produces the film of interest, normally through a numerical optimization procedure. We refer to the combination of kinetic and reactor models as a fundamental model to distinguish it from empirical, linear models determined directly from reactor data. The primary disadvantage of the empirical, statistical models is that they are accurate only in a restricted regime of the operating space and must be re-identified when the device structure changes. An advantage of the fundamental model based approach is its great flexibility in allowing new and unusual film profiles. All of the effort is expended in capturing the relevant chemistries in the kinetic models; little effort is required to determine the optimal recipe for each new film profile encountered. Because the model provides a reasonably accurate road-map for each new film considered, the time required for experimental verification of the final operating policy is greatly reduced.

Relevance to DoD

This research program developed a manufacturing process to produce device structures that are unattainable or unaffordable with today's commercial manufacturing methods. This will impact on DoD operations through the development of an intelligent manufacturing process for growth of novel alloy films and fabrication of application specific integrated circuits that seek to take advantage of the band gap and band edge manipulation afforded by the Si-Ge-C ternary system. This program will enable rapid development and manufacturing of low power, high-speed application specific integrated circuits by moving thermal chemical vapor deposition away from recipe driven growth to one that is fully controlled. To our knowledge no manufacturer has adopted the technology developed in the program so the impact on DoD remains more promise than fact. In a similar vein, patents were filed and separately sponsored research with commercial entities that was a direct consequence of the DoD research program can be cited; however, these illustrations of technology transfer do not lead directly to a process, product or technology innovation being directly used by DoD.

Productivity

Over the period of funding a total of 68 articles appeared in archival journals or conference proceedings and 116 talks were presented at topical conferences and national and international technical meetings. Additional articles continue to be published. The principal investigators were recognized by professional societies: three were made fellows of societies (IEEE and APS) and one received a National research award for contributions to the growth of electronic and photonic materials. The principal investigators were recognized by National lectureships, and one received a Semiconductor Research Inventor's award for work on electronic devices. Finally, several investigators were recognized by their home institutions with endowed professorships or lectureships.

Student Involvement

Over the period of the funding a total of nine postdoctoral associates were supported and 22 graduate students were supported. Over half of these graduate students earned Ph.D. degrees. These students are now working in organizations principally in the microelectronics industry at companies including: Cypress Semiconductor, Intel Corporation, Motorola Inc., KLA, IBM, Ball Semiconductor, Texas Instruments, Applied Materials, and Advanced Micro Devices. Perhaps the greatest benefit was working on interdisciplinary programs and having access to more than one supervising professor over the course of the research. Students have always commented on the positive benefits of interdisciplinary efforts and how this better prepared them to contribute once they leave a university setting. Some students also enjoyed working a project with a grand vision and seeing how their component was ultimately used to make the entire project a success.